Analysis of Packing Function Solutions for Monomeric Proteins

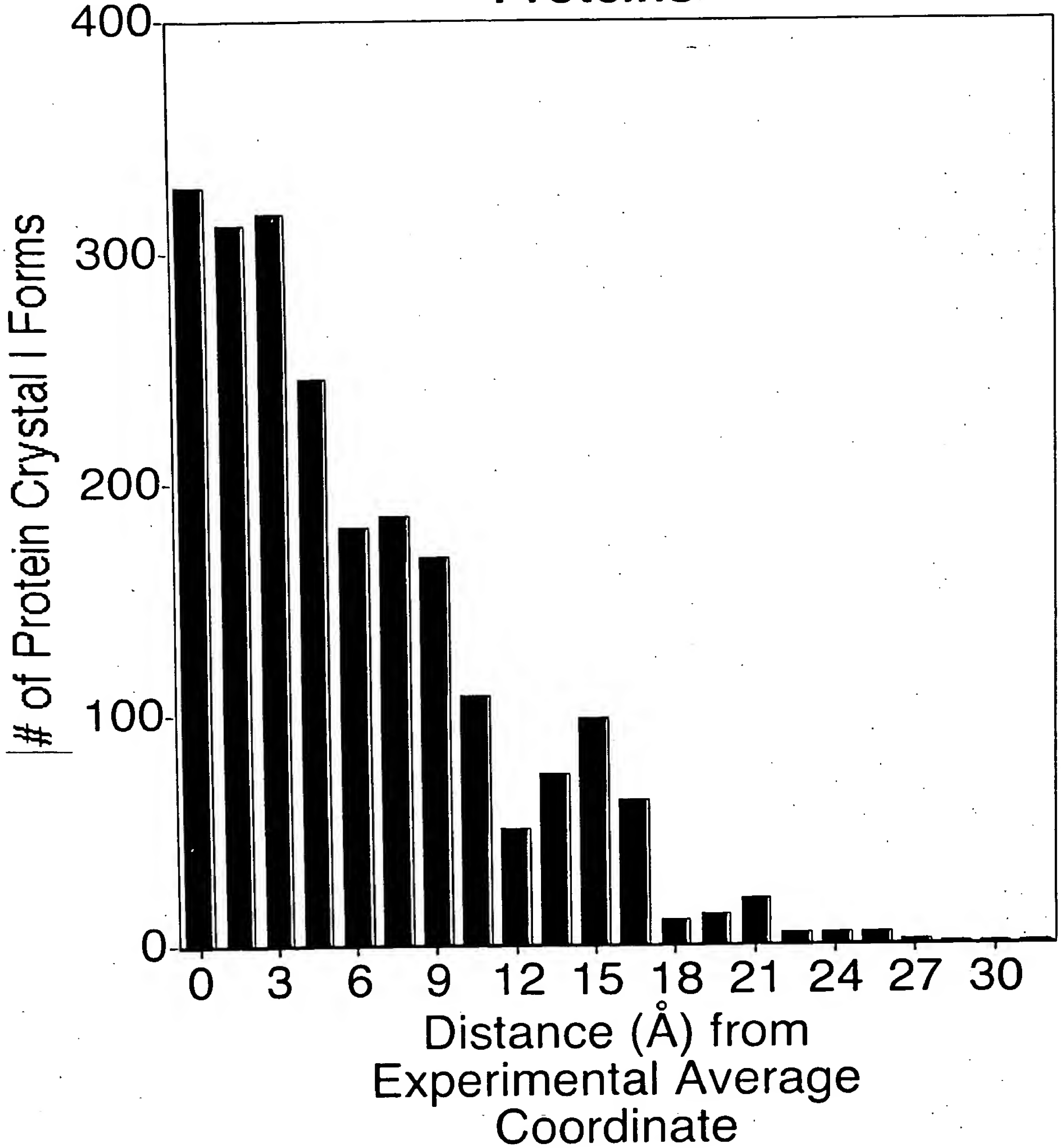


FIG. 1

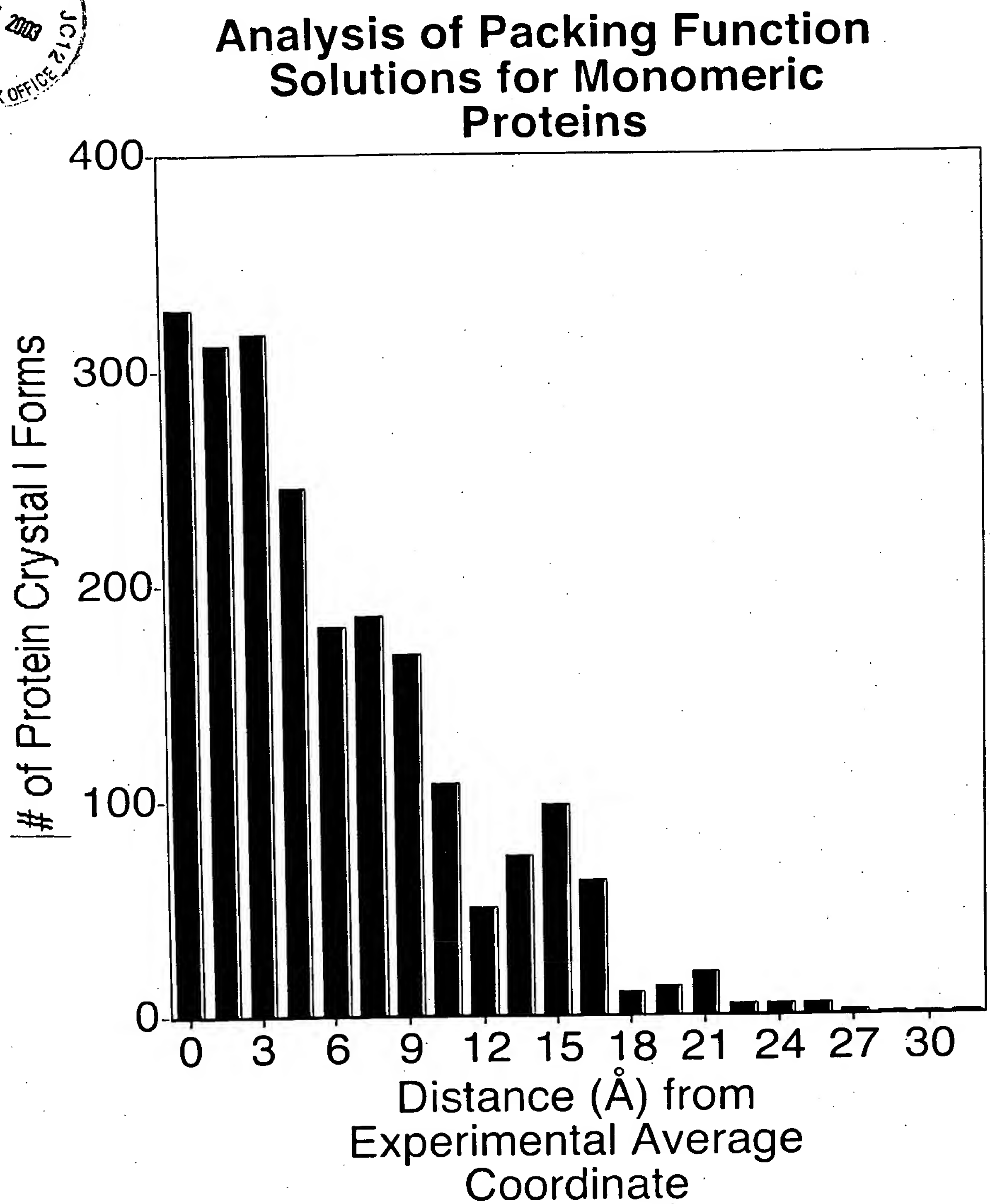

Analysis of Packing Function Solutions for Monomeric Proteins
400
300
200
100
0
# of Protein Crystal l Forms
0 3 6 9 12 15 18 21 24 27 30
Distance (Å) from Experimental Average Coordinate

FIG. 2

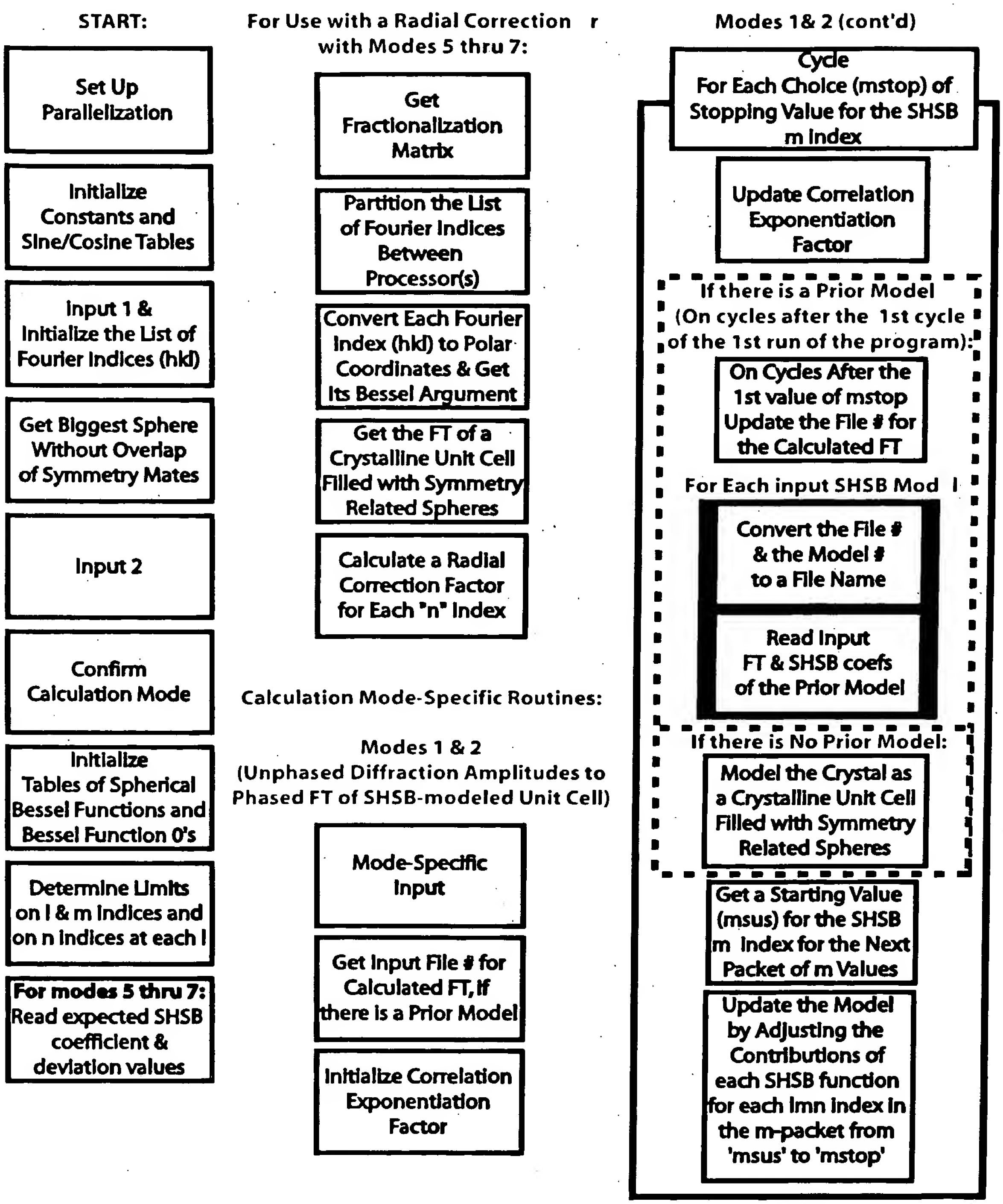

START:
Set Up Parallelization
Initialize Constants and Sine/Cosine Tables
Input 1 & Initialize the List of Fourier Indices (hkl)
Get Biggest Sphere Without Overlap of Symmetry Mates
Input 2
Confirm Calculation Mode
Initialize Tables of Spherical Bessel Functions and Bessel Function 0's
Determine Limits on l & m Indices and on n Indices at each l
For modes 5 thru 7: Read expected SHSB coefficient & deviation values
For Use with a Radial Correction r with Modes 5 thru 7:
Get Fractionalization Matrix
Partition the List of Fourier Indices Between Processor(s)
Convert Each Fourier Index (hkl) to Polar Coordinates & Get Its Bessel Argument
Get the FT of a Crystalline Unit Cell Filled with Symmetry Related Spheres
Calculate a Radial Correction Factor for Each "n" Index
Calculation Mode-Specific Routines:
Modes 1 & 2
(Unphased Diffraction Amplitudes to Phased FT of SHSB-modeled Unit Cell)
Mode-Specific Input
Get Input File # for Calculated FT, if there is a Prior Model
Initialize Correlation Exponentiation Factor
Modes 1& 2 (cont'd)
Cycle
For Each Choice (mstop) of Stopping Value for the SHSB m Index
Update Correlation Exponentiation Factor
If there is a Prior Model
(On cycles after the 1st cycle of the 1st run of the program):
On Cycles After the 1st value of mstop Update the File # for the Calculated FT
For Each input SHSB Mod l
Convert the File # & the Model # to a File Name
Read Input FT & SHSB coefs of the Prior Model
If there is No Prior Model:
Model the Crystal as a Crystalline Unit Cell Filled with Symmetry Related Spheres
Get a Starting Value (msus) for the SHSB m Index for the Next Packet of m Values
Update the Model by Adjusting the Contributions of each SHSB function for each lmn index in the m-packet from 'msus' to 'mstop'

FIG. 3

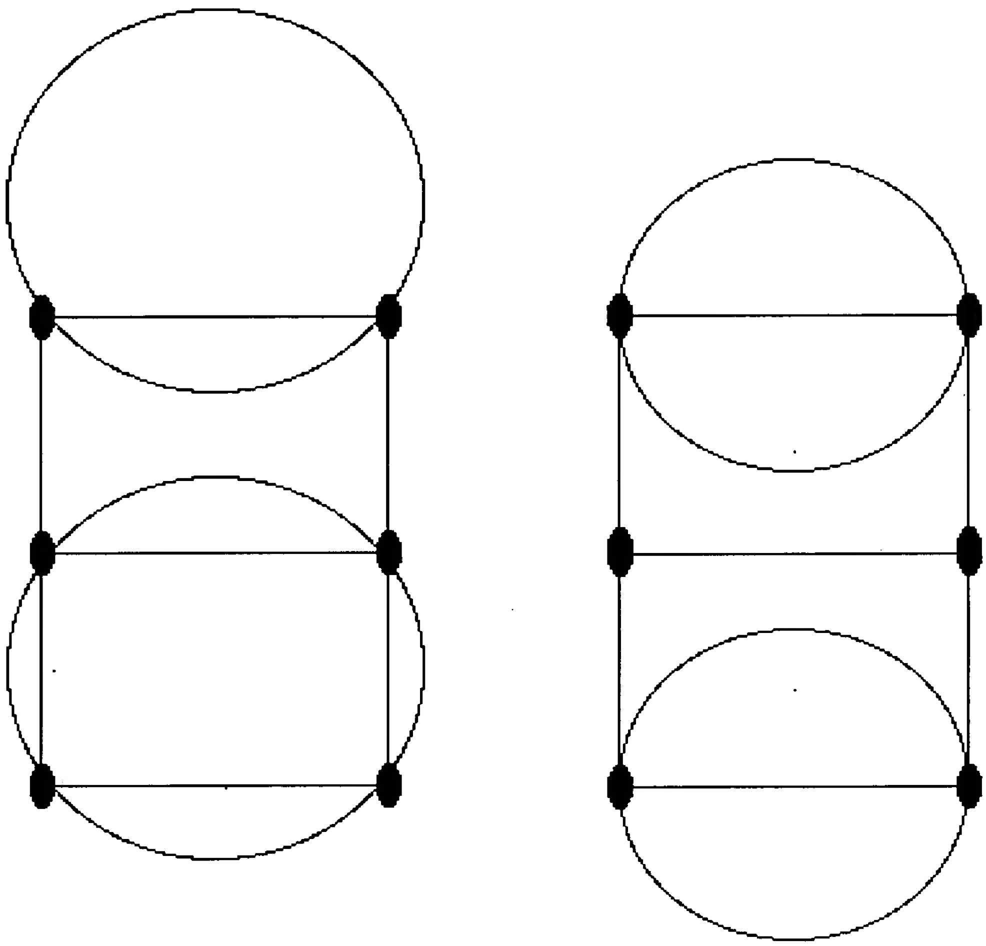


Figure . A schematic example: Two choices for filling the same portion of a crystal unit cell from an orthorhombic Spacegroup. Although the spheres on the right are smaller than those on the left, for some crystals the local maximum in the packing on the right would be the packing of maximal consistency with the crystallographic data.

FIG. 4

Initialize Fractionalization Matrix

Initialize the Equal Partitioning of the Fourier (hkl) Index between Processors

On 1st Cycle of 1st Run:
Prescale Observed Diffraction to that of a Unit Cell of Spheres

Define the First SHSB Index Triplet (lmn) for which to Consider Model |F|'s

Initialize for Index-by-Index Update of Origin-Centered SHSB Basis Function

Modes 4 & 5 only:
Initialize Buffers for Cumulative Update of Fourier Representation

Initialize Pointers to Stored Fourier Representations of Model and of Basis

Mode 3 only:
Get File Name from File # & Open It to Let SHSB Coefs. be Read

For each "m" Index (0 to maximum "m")

For Each hkl in this Partition:
Update "m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "l" Index (present "m" to maximum "l")

For Each hkl in this Partition:
Update "l,m" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

For each "n" Index (1 to maximum "n" for each "l")

For Each hkl in this Partition:
Update "n" Recursion Formula for Fourier Representation of the Origin-Centered SHSB

Depending on Mode:
Choose the # of Passes and # of Presumed Phase Angles Needed for the SHSB coef. with this SHSB index (lmn)

Set the Presumed Amplitude of the Origin-Centered SHSB Basis Function

FIRST PASS:
Initialize Registers: Overall Comparison of Correlation Coef. & Other Statistics

Renitialize Pointers to Storage Sites for Fourier Representations of the Full-Unit-Cell SHSB Basis

Parallel Processor Version:

Set # of calculations to: (# of presumed values of SHSB coef.'s phase) X (# of stored accumulated SHSB models for trial combination with this new SHSB component)

Given: # of processors # of hkl partitions # of calculations **Get:** # of required rounds of trial combinations

For each round of trial combination on this processor

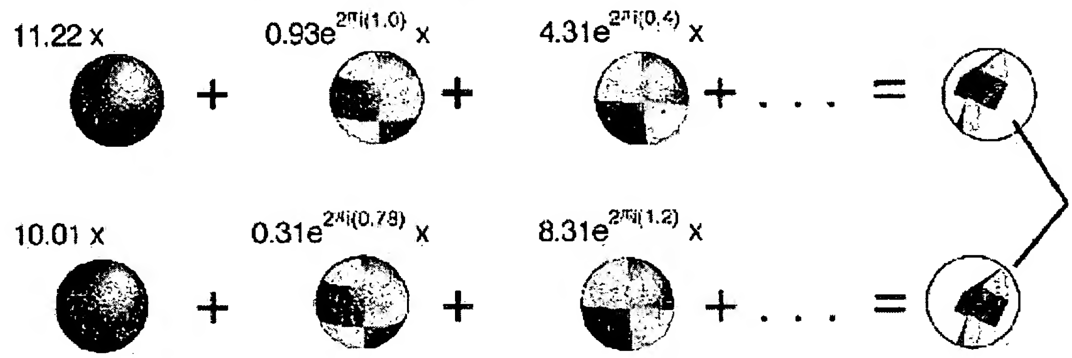
Single Processor Version: (Outer Loop)

For each presumed value of the SHSB coef.'s phase

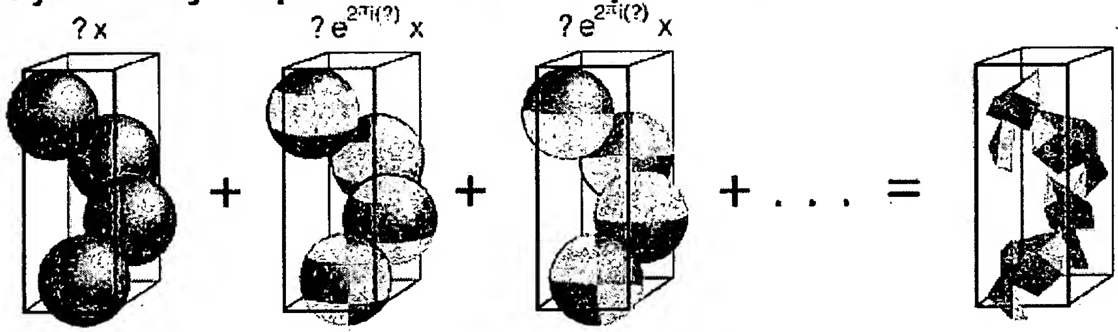
Initialize Registers: Angular Comparison of Correlation Coef. & Other Statistics

FIG. 5

Identical Image from Expansions about Different Origins:



Symmetry Expanded Direct Space Basis Functions:



With a properly chosen origin, 45-55% of the unit cell can be expanded. (Most protein crystals are > 45% solvent.)

FIG. 6

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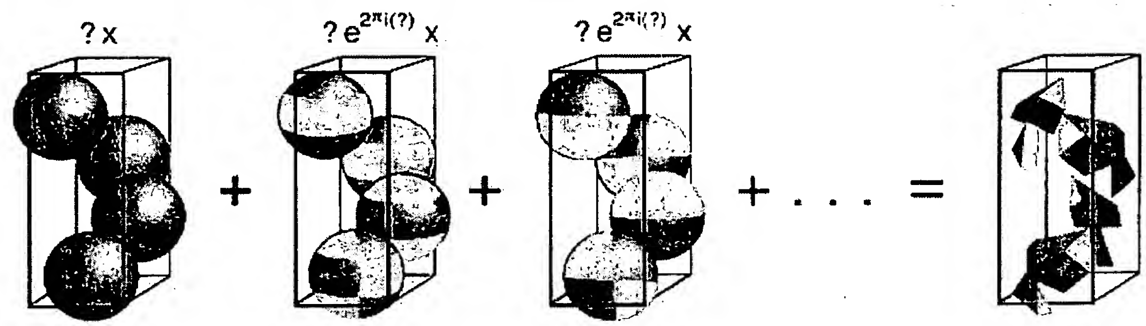
Component Direct Space Basis Functions:



Component Fourier Transforms:

$$a_{001} F_{solo}^{001}(hkl) + a_{211} F_{solo}^{211}(hkl) + a_{111} F_{solo}^{111}(hkl) + \ldots = F_{obs}(hkl)$$

$$a_{001} = \Sigma_{hkl} F^{*}{}_{solo}^{001}(hkl)\, F_{obs}(hkl) \quad \text{[presume } \phi = 0.00 \text{ to start]}$$

$$F_{accum}(hkl) = a_{001} F_{solo}^{001}(hkl)$$

$$a_{211} = \Sigma_{hkl} F^{*}{}_{solo}^{211}(hkl) \left(|F_{obs}(hkl)| - |F^{n}_{accum}(hkl)|\right) e^{2\pi i \phi^{n}_{accum}(hkl)}$$

$$F^{n+1}_{accum}(hkl) = F^{n}_{accum}(hkl) + a_{211} F_{solo}^{211}(hkl)$$

FIG. 7